Full wwPDB X-ray Structure Validation Report

Aug 29, 2020 – 02:50 PM BST

PDB ID	:	4N2O
Title	:	Structure of a novel autonomous cohesin protein from Ruminococcus flavefaciens
Authors	:	Frolow, F.; Voronov-Goldman, M.; Levy-Assaraf, M.; Lamed, R.; Bayer, E.; Shimon, L.
Deposited on	:	2013-10-05
Resolution	:	2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

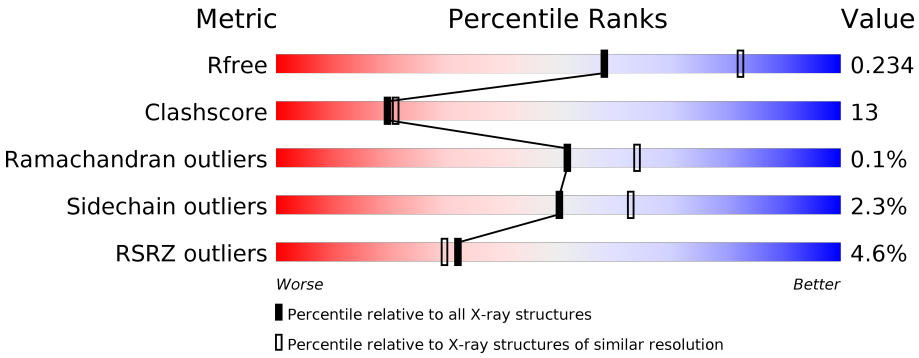
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	201	5% 81% 14%
1	B	201	4% 80% 14%
1	C	201	4% 79% 14% 5%
1	D	201	7% 81% 13% 5%
1	E	201	3% 80% 13% 5%
1	F	201	6% 78% 16%

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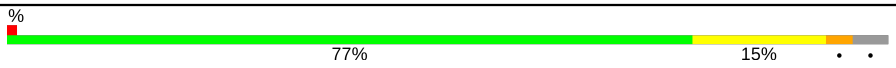
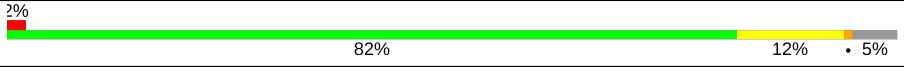
Mol	Chain	Length	Quality of chain
1	G	201	
1	H	201	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	H	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Autonomous cohesin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	Se	0	0	0
			1499	941	240	304	3	11			
1	B	193	Total	C	N	O	S	Se	0	0	0
			1489	936	238	301	3	11			
1	C	190	Total	C	N	O	S	Se	0	0	0
			1473	927	237	295	3	11			
1	D	191	Total	C	N	O	S	Se	0	0	0
			1470	925	234	297	3	11			
1	E	190	Total	C	N	O	S	Se	0	0	0
			1467	924	233	296	3	11			
1	F	193	Total	C	N	O	S	Se	0	1	0
			1508	948	245	300	3	12			
1	G	192	Total	C	N	O	S	Se	0	1	0
			1491	938	238	300	3	12			
1	H	191	Total	C	N	O	S	Se	0	1	0
			1485	935	237	298	3	12			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		

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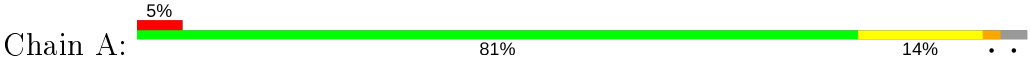
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	58	Total O 58 58	0	0
3	C	51	Total O 51 51	0	0
3	D	6	Total O 6 6	0	0
3	E	8	Total O 8 8	0	0
3	F	53	Total O 53 53	0	0
3	G	69	Total O 69 69	0	0
3	H	64	Total O 64 64	0	0

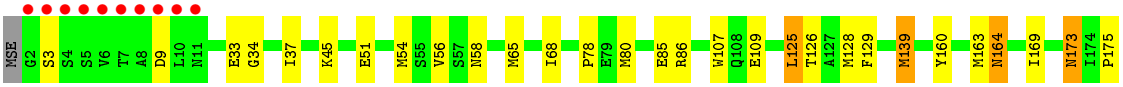
3 Residue-property plots (i)

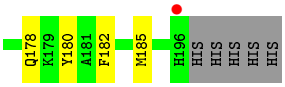
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Autonomous cohesin

Chain A:

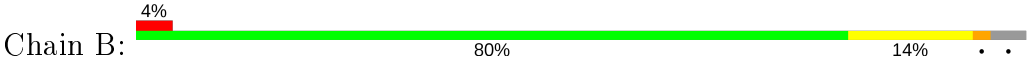


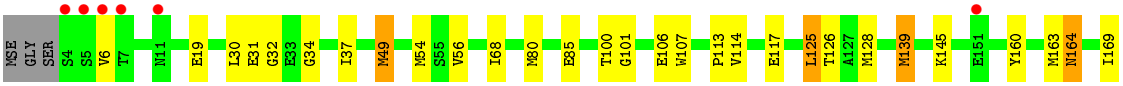


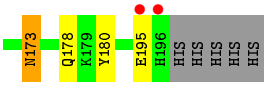


- Molecule 1: Autonomous cohesin

Chain B:

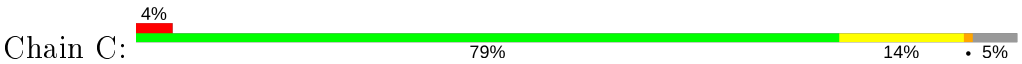


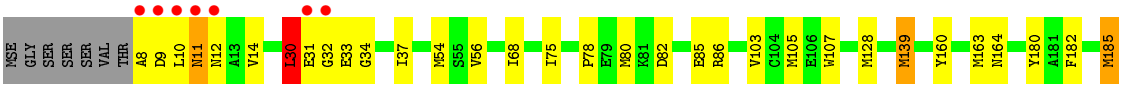


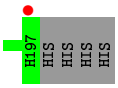


- Molecule 1: Autonomous cohesin

Chain C:

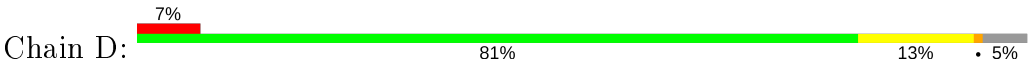


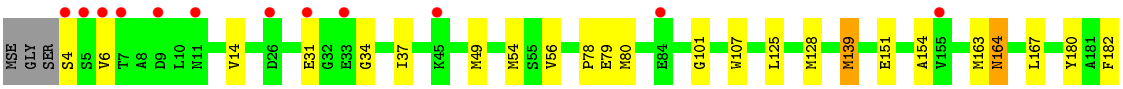


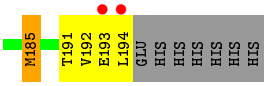


- Molecule 1: Autonomous cohesin

Chain D:

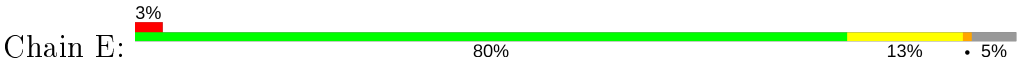


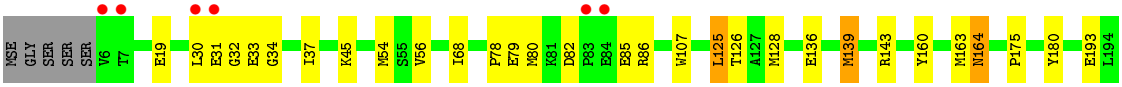




• Molecule 1: Autonomous cohesin

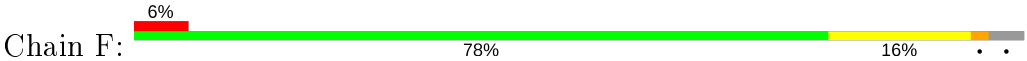
Chain E:

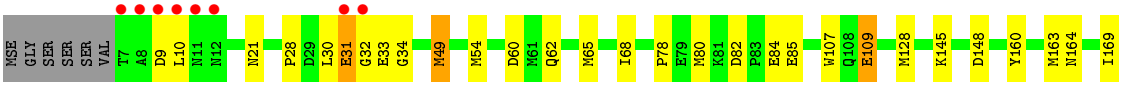


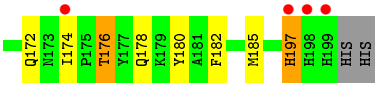


• Molecule 1: Autonomous cohesin

Chain F:

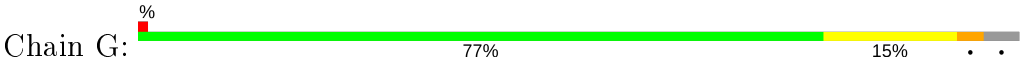


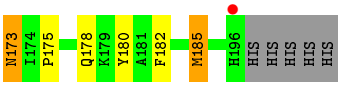




• Molecule 1: Autonomous cohesin

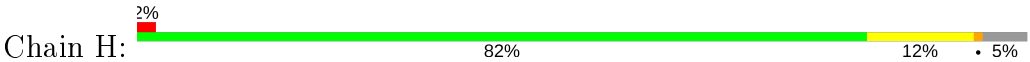
Chain G:

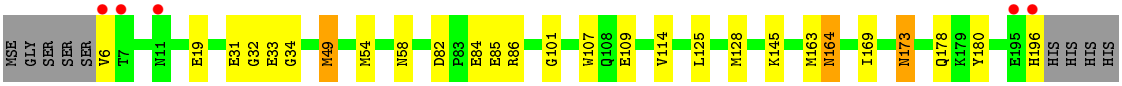




• Molecule 1: Autonomous cohesin

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.24Å 67.73Å 258.91Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	22.77 – 2.44 22.77 – 2.44	Depositor EDS
% Data completeness (in resolution range)	96.8 (22.77-2.44) 91.0 (22.77-2.44)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.8.0049, PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.229 0.213 , 0.234	Depositor DCC
R_{free} test set	3683 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.025 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/1520	0.78	2/2045 (0.1%)
1	B	0.58	0/1510	0.75	2/2032 (0.1%)
1	C	0.56	0/1495	0.78	3/2011 (0.1%)
1	D	0.52	0/1490	0.78	2/2005 (0.1%)
1	E	0.56	0/1487	0.80	3/2001 (0.1%)
1	F	0.57	0/1532	0.83	1/2061 (0.0%)
1	G	0.62	0/1512	0.83	4/2034 (0.2%)
1	H	0.55	0/1506	0.74	1/2026 (0.0%)
All	All	0.57	0/12052	0.79	18/16215 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	49	MSE	CG-SE-CE	9.33	119.42	98.90
1	G	49	MSE	CG-SE-CE	8.54	117.70	98.90
1	B	49	MSE	CG-SE-CE	7.51	115.43	98.90
1	D	185	MSE	CG-SE-CE	-7.43	82.56	98.90
1	C	185	MSE	CG-SE-CE	-7.37	82.69	98.90
1	H	49	MSE	CG-SE-CE	7.29	114.94	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	185	MSE	CA-CB-CG	6.94	125.10	113.30
1	A	139	MSE	CG-SE-CE	6.31	112.79	98.90
1	B	139	MSE	CG-SE-CE	6.14	112.41	98.90
1	G	139	MSE	CG-SE-CE	6.14	112.41	98.90
1	C	139	MSE	CG-SE-CE	5.81	111.69	98.90
1	A	9	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	30	LEU	N-CA-CB	5.70	121.81	110.40
1	C	30	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	139	MSE	CG-SE-CE	5.53	111.07	98.90
1	E	139	MSE	CG-SE-CE	5.43	110.85	98.90
1	G	185	MSE	CG-SE-CE	5.38	110.74	98.90
1	E	136	GLU	N-CA-CB	-5.03	101.54	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	ASN	Peptide
1	C	12	ASN	Peptide
1	G	10	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1499	0	1420	44	0
1	B	1489	0	1412	51	0
1	C	1473	0	1393	39	0
1	D	1470	0	1399	39	0
1	E	1467	0	1395	32	0
1	F	1508	0	1422	55	0
1	G	1491	0	1415	47	0
1	H	1485	0	1410	36	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
2	H	1	0	0	2	0
3	A	74	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	58	0	0	3	0
3	C	51	0	0	1	0
3	D	6	0	0	1	0
3	E	8	0	0	0	0
3	F	53	0	0	0	0
3	G	69	0	0	5	0
3	H	64	0	0	2	0
All	All	12269	0	11266	294	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128[B]:MSE:HG3	1:H:128[B]:MSE:CE	1.55	1.36
1:A:128:MSE:HE3	1:A:129:PHE:O	1.23	1.29
1:G:128[B]:MSE:CG	1:H:128[B]:MSE:HE3	1.71	1.18
1:F:49:MSE:HE2	1:F:145:LYS:HD3	1.33	1.10
1:B:49:MSE:HE2	1:B:145:LYS:HD3	1.13	1.08
1:H:49:MSE:HE2	1:H:145:LYS:HD3	1.13	1.06
3:G:368:HOH:O	1:H:86:ARG:HD2	1.53	1.06
1:G:49:MSE:HE2	1:G:145:LYS:HD3	1.35	1.02
1:B:49:MSE:CE	1:B:145:LYS:HD3	1.88	1.01
1:H:49:MSE:CE	1:H:145:LYS:HD3	1.89	1.00
1:G:182:PHE:HA	1:G:185:MSE:HE3	1.39	1.00
1:B:49:MSE:HE2	1:B:145:LYS:CD	1.96	0.96
1:C:54:MSE:HE3	1:C:160:TYR:HE1	1.28	0.95
1:E:54:MSE:HE3	1:E:160:TYR:HE1	1.29	0.95
1:H:49:MSE:HE2	1:H:145:LYS:CD	1.96	0.95
1:F:54:MSE:HE3	1:F:160:TYR:HE1	1.29	0.94
1:A:54:MSE:HE3	1:A:160:TYR:HE1	1.28	0.94
1:B:54:MSE:HE3	1:B:160:TYR:HE1	1.30	0.93
1:C:56:VAL:HB	1:C:139:MSE:HE2	1.51	0.92
1:A:56:VAL:HB	1:A:139:MSE:HE2	1.51	0.91
1:A:54:MSE:CE	1:A:160:TYR:HE1	1.84	0.91
1:G:56:VAL:HB	1:G:139:MSE:HE2	1.51	0.90
1:E:56:VAL:HB	1:E:139:MSE:HE2	1.53	0.90
1:B:56:VAL:HB	1:B:139:MSE:HE2	1.53	0.89
1:D:56:VAL:HB	1:D:139:MSE:HE2	1.52	0.89
1:G:128[B]:MSE:CG	1:H:128[B]:MSE:CE	2.38	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:MSE:CE	1:C:160:TYR:HE1	1.88	0.87
1:C:31:GLU:HG3	1:C:31:GLU:O	1.72	0.86
1:A:128:MSE:CE	1:A:129:PHE:O	2.19	0.86
1:B:54:MSE:CE	1:B:160:TYR:HE1	1.87	0.86
1:E:54:MSE:CE	1:E:160:TYR:HE1	1.87	0.86
1:F:54:MSE:CE	1:F:160:TYR:HE1	1.90	0.85
1:C:8:ALA:HB3	1:C:10:LEU:N	1.92	0.81
1:C:182:PHE:O	1:C:185:MSE:HE2	1.81	0.81
1:D:182:PHE:O	1:D:185:MSE:HE2	1.81	0.79
1:F:9:ASP:C	1:F:10:LEU:HD23	2.02	0.79
1:C:54:MSE:HE1	1:C:68:ILE:HG21	1.64	0.79
1:D:151:GLU:O	1:D:192:VAL:HG11	1.82	0.79
1:A:109:GLU:OE2	1:B:19:GLU:HG2	1.83	0.78
1:G:19:GLU:HG2	1:H:109:GLU:OE2	1.83	0.78
1:A:54:MSE:CE	1:A:160:TYR:CE1	2.66	0.78
1:E:54:MSE:HE1	1:E:68:ILE:HG21	1.65	0.78
1:E:54:MSE:CE	1:E:160:TYR:CE1	2.67	0.78
1:B:54:MSE:HE1	1:B:68:ILE:HG21	1.64	0.77
1:F:54:MSE:HE1	1:F:68:ILE:HG21	1.66	0.77
1:B:54:MSE:CE	1:B:160:TYR:CE1	2.68	0.77
1:C:8:ALA:N	1:C:9:ASP:HA	1.99	0.77
1:A:54:MSE:HE1	1:A:68:ILE:HG21	1.66	0.76
1:C:54:MSE:CE	1:C:160:TYR:CE1	2.68	0.75
1:F:54:MSE:CE	1:F:160:TYR:CE1	2.68	0.75
2:H:301:CL:CL	3:H:436:HOH:O	2.43	0.72
2:H:301:CL:CL	3:H:430:HOH:O	2.43	0.72
1:G:128[A]:MSE:SE	1:H:128[A]:MSE:CB	2.88	0.71
1:F:49:MSE:CE	1:F:145:LYS:HD3	2.18	0.71
2:A:301:CL:CL	3:A:446:HOH:O	2.46	0.71
1:E:85:GLU:O	1:E:86:ARG:HG3	1.90	0.70
1:G:109:GLU:OE2	1:H:19:GLU:HG2	1.90	0.70
1:G:85:GLU:OE2	1:H:173:ASN:ND2	2.24	0.69
1:G:128[A]:MSE:SE	1:H:128[A]:MSE:HB2	2.43	0.69
1:G:128[B]:MSE:HG3	1:H:128[B]:MSE:HE3	0.77	0.68
1:A:85:GLU:OE2	1:B:173:ASN:ND2	2.26	0.68
1:G:182:PHE:HA	1:G:185:MSE:CE	2.21	0.68
1:B:80:MSE:HE2	3:B:422:HOH:O	1.93	0.68
1:G:9:ASP:N	1:G:9:ASP:OD1	2.26	0.67
1:A:128:MSE:HB2	1:B:128:MSE:SE	2.45	0.67
1:G:128[A]:MSE:SE	1:H:128[A]:MSE:HB3	2.45	0.67
1:F:9:ASP:O	1:F:10:LEU:HD23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLU:CD	1:F:28:PRO:HB3	2.16	0.66
1:G:182:PHE:CG	1:G:185:MSE:HE3	2.30	0.66
1:F:172:GLN:HG2	1:F:174:ILE:HG12	1.76	0.66
1:A:78:PRO:HB2	1:A:80:MSE:CE	2.26	0.66
1:B:49:MSE:HE3	1:C:82:ASP:CG	2.17	0.65
1:F:78:PRO:HB2	1:F:80:MSE:CE	2.27	0.64
1:A:78:PRO:HG2	1:A:80:MSE:CE	2.28	0.64
1:C:54:MSE:HE3	1:C:160:TYR:CE1	2.20	0.64
1:G:128[A]:MSE:HE3	1:H:128[A]:MSE:HE2	1.79	0.64
1:F:54:MSE:HE3	1:F:160:TYR:CE1	2.21	0.64
1:F:33:GLU:HG2	1:F:180:TYR:OH	1.98	0.64
1:F:78:PRO:HG2	1:F:80:MSE:CE	2.28	0.64
1:C:78:PRO:HG2	1:C:80:MSE:CE	2.29	0.63
1:D:151:GLU:O	1:D:192:VAL:CG1	2.46	0.63
1:C:78:PRO:HB2	1:C:80:MSE:CE	2.29	0.63
1:C:33:GLU:HG2	1:C:180:TYR:OH	1.98	0.63
1:E:82:ASP:OD2	1:E:85:GLU:CD	2.37	0.63
1:B:34:GLY:HA3	1:B:180:TYR:CE1	2.34	0.63
1:B:6:VAL:HG21	1:B:114:VAL:HA	1.79	0.63
1:F:65:MSE:HE3	1:F:128[B]:MSE:HG2	1.81	0.62
1:F:28:PRO:O	1:F:176:THR:OG1	2.16	0.62
1:D:78:PRO:HG2	1:D:80:MSE:CE	2.30	0.62
1:C:31:GLU:CG	1:C:31:GLU:O	2.48	0.61
1:G:49:MSE:CE	1:G:145:LYS:HD3	2.20	0.61
1:G:182:PHE:O	1:G:185:MSE:HG2	2.00	0.61
1:D:31:GLU:OE1	1:D:31:GLU:HA	2.00	0.61
1:D:192:VAL:O	1:D:193:GLU:HB2	2.01	0.61
1:D:78:PRO:HB2	1:D:80:MSE:CE	2.30	0.61
1:E:78:PRO:HB2	1:E:80:MSE:CE	2.30	0.61
1:D:79:GLU:OE1	1:F:28:PRO:HB3	2.01	0.60
1:E:78:PRO:HG2	1:E:80:MSE:CE	2.31	0.60
1:G:61:MSE:CE	3:G:346:HOH:O	2.49	0.60
1:A:37:ILE:HG23	1:A:139:MSE:HE1	1.83	0.60
1:E:85:GLU:O	1:E:86:ARG:CG	2.49	0.60
1:A:128:MSE:CB	1:B:128:MSE:SE	3.00	0.60
1:B:34:GLY:CA	1:B:180:TYR:CD1	2.85	0.60
1:B:49:MSE:HE1	1:B:145:LYS:HB2	1.82	0.60
1:E:37:ILE:HG23	1:E:139:MSE:HE1	1.84	0.60
1:C:37:ILE:HG23	1:C:139:MSE:HE1	1.84	0.59
1:G:182:PHE:CA	1:G:185:MSE:HE3	2.23	0.59
1:B:37:ILE:HG23	1:B:139:MSE:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:ILE:HG23	1:G:139:MSE:HE1	1.85	0.58
1:D:37:ILE:HG23	1:D:139:MSE:HE1	1.85	0.58
1:A:65:MSE:HE3	1:B:128:MSE:HE1	1.86	0.58
1:D:154:ALA:N	1:D:192:VAL:HG12	2.19	0.57
1:C:86:ARG:NH2	1:D:164:ASN:O	2.37	0.57
1:B:80:MSE:HE1	1:B:106:GLU:CD	2.25	0.57
1:H:49:MSE:HE1	1:H:145:LYS:HB2	1.85	0.57
1:E:54:MSE:HE3	1:E:160:TYR:CE1	2.21	0.57
1:E:33:GLU:HB2	1:E:180:TYR:CZ	2.40	0.57
1:G:6:VAL:HG22	1:G:29:ASP:OD1	2.05	0.57
1:B:6:VAL:HG11	1:B:113:PRO:HB2	1.86	0.56
1:A:78:PRO:HG2	1:A:80:MSE:HE1	1.88	0.56
1:D:79:GLU:HG2	1:F:28:PRO:CG	2.36	0.56
1:C:78:PRO:HG2	1:C:80:MSE:HE1	1.88	0.56
1:G:45:LYS:HE2	3:G:359:HOH:O	2.06	0.56
1:A:78:PRO:O	1:A:80:MSE:HE3	2.07	0.55
1:B:126:THR:CG2	1:B:128:MSE:HE2	2.36	0.54
1:F:82:ASP:CG	1:H:49:MSE:HE3	2.28	0.54
1:G:86:ARG:HD3	3:G:369:HOH:O	2.07	0.54
1:F:78:PRO:HG2	1:F:80:MSE:HE1	1.90	0.54
1:C:78:PRO:O	1:C:80:MSE:HE3	2.07	0.54
1:E:79:GLU:OE1	1:E:143:ARG:HD3	2.07	0.54
1:D:78:PRO:HG2	1:D:80:MSE:HE1	1.89	0.54
1:A:65:MSE:CE	1:B:128:MSE:HE1	2.38	0.53
1:D:78:PRO:O	1:D:80:MSE:HE3	2.08	0.53
1:G:173:ASN:ND2	1:H:85:GLU:OE2	2.42	0.53
1:E:128:MSE:SE	1:F:128[B]:MSE:SE	3.26	0.53
1:E:78:PRO:HG2	1:E:80:MSE:HE1	1.90	0.53
1:E:45:LYS:HA	1:E:193:GLU:O	2.09	0.53
1:F:30:LEU:CD1	1:F:176:THR:CG2	2.87	0.53
1:F:30:LEU:CD1	1:F:176:THR:HG23	2.39	0.53
1:F:78:PRO:HG2	1:F:80:MSE:HE3	1.91	0.53
1:E:78:PRO:O	1:E:80:MSE:HE3	2.09	0.53
1:F:78:PRO:O	1:F:80:MSE:HE3	2.09	0.52
1:C:128:MSE:HE2	1:D:128:MSE:HE3	1.90	0.52
1:B:80:MSE:HE3	3:B:416:HOH:O	2.09	0.52
1:A:54:MSE:HG2	1:A:139:MSE:HE3	1.92	0.52
1:C:30:LEU:CD2	1:C:31:GLU:N	2.72	0.52
1:F:169:ILE:HG23	1:F:178:GLN:OE1	2.10	0.52
1:F:65:MSE:SE	1:F:128[B]:MSE:HE3	2.59	0.52
1:B:80:MSE:HE1	1:B:106:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HG2	1:A:80:MSE:HE3	1.91	0.51
1:E:128:MSE:SE	1:F:128[B]:MSE:HG3	2.61	0.51
1:G:169:ILE:HG23	1:G:178:GLN:OE1	2.10	0.51
1:B:169:ILE:HG23	1:B:178:GLN:OE1	2.10	0.51
1:F:30:LEU:HD13	1:F:176:THR:HG23	1.91	0.51
1:C:78:PRO:HG2	1:C:80:MSE:HE3	1.93	0.51
1:G:54:MSE:HG2	1:G:139:MSE:HE3	1.92	0.51
1:E:34:GLY:HA3	1:E:180:TYR:CE1	2.46	0.51
1:B:54:MSE:HG2	1:B:139:MSE:HE3	1.93	0.51
1:A:51:GLU:OE2	3:A:472:HOH:O	2.19	0.51
1:G:49:MSE:HE1	1:G:145:LYS:HB2	1.93	0.51
1:H:169:ILE:HG23	1:H:178:GLN:OE1	2.10	0.51
1:F:10:LEU:HD23	1:F:10:LEU:N	2.24	0.50
1:E:19:GLU:O	1:F:109:GLU:OE2	2.30	0.50
1:C:54:MSE:HG2	1:C:139:MSE:HE3	1.93	0.50
1:A:169:ILE:HG23	1:A:178:GLN:OE1	2.11	0.50
1:A:78:PRO:CB	1:A:80:MSE:CE	2.89	0.50
1:F:30:LEU:HD12	1:F:176:THR:CG2	2.41	0.50
1:A:173:ASN:ND2	1:B:85:GLU:OE2	2.45	0.50
1:D:54:MSE:HG2	1:D:139:MSE:HE3	1.93	0.50
1:D:79:GLU:CG	1:F:28:PRO:HD3	2.42	0.50
1:D:4:SER:HB3	1:D:6:VAL:HG22	1.93	0.49
1:C:30:LEU:HD22	1:C:31:GLU:N	2.27	0.49
1:B:54:MSE:HE3	1:B:160:TYR:CE1	2.23	0.49
1:E:54:MSE:HG2	1:E:139:MSE:HE3	1.94	0.49
1:A:128:MSE:HE2	1:B:100:THR:C	2.33	0.49
1:D:78:PRO:HG2	1:D:80:MSE:HE3	1.94	0.48
1:A:86:ARG:NH2	1:B:164:ASN:O	2.46	0.48
1:F:78:PRO:CB	1:F:80:MSE:CE	2.91	0.48
1:A:128:MSE:SE	1:B:101:GLY:HA3	2.63	0.48
1:C:78:PRO:CB	1:C:80:MSE:CE	2.92	0.48
1:D:79:GLU:HG2	1:F:28:PRO:HG3	1.95	0.48
1:A:45:LYS:HE2	3:A:467:HOH:O	2.13	0.48
1:A:107:TRP:CH2	1:A:163:MSE:HE1	2.49	0.48
1:E:78:PRO:HG2	1:E:80:MSE:HE3	1.94	0.48
1:G:101:GLY:HA3	1:H:128[A]:MSE:SE	2.64	0.48
1:A:54:MSE:HE3	1:A:160:TYR:CE1	2.21	0.48
1:H:34:GLY:HA3	1:H:180:TYR:CE1	2.49	0.48
1:G:107:TRP:CH2	1:G:163:MSE:HE1	2.49	0.48
1:G:175:PRO:HG3	1:H:85:GLU:HB2	1.96	0.48
1:F:34:GLY:HA3	1:F:180:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:MSE:CE	1:H:125:LEU:HD22	2.44	0.47
1:B:126:THR:HG21	1:B:128:MSE:HE2	1.96	0.47
1:D:78:PRO:CB	1:D:80:MSE:CE	2.93	0.47
1:E:107:TRP:CH2	1:E:163:MSE:HE1	2.50	0.47
1:B:34:GLY:HA2	1:B:180:TYR:CD1	2.50	0.47
1:D:128:MSE:HB3	3:D:305:HOH:O	2.14	0.47
1:G:8:ALA:HA	1:G:10:LEU:HD12	1.97	0.47
1:G:86:ARG:NH2	1:H:164:ASN:O	2.48	0.47
1:A:175:PRO:HG3	1:B:85:GLU:HB2	1.97	0.47
1:C:14:VAL:CG2	1:C:185:MSE:CE	2.93	0.47
1:D:107:TRP:CH2	1:D:163:MSE:HE1	2.50	0.47
1:E:175:PRO:HG2	1:F:84:GLU:HG3	1.97	0.46
1:A:128:MSE:HB3	1:B:128:MSE:SE	2.65	0.46
1:B:31:GLU:HA	1:B:32:GLY:HA2	1.65	0.46
1:D:34:GLY:HA3	1:D:180:TYR:CE1	2.50	0.46
1:A:85:GLU:O	1:A:85:GLU:HG3	2.16	0.46
1:C:103:VAL:HG23	3:C:339:HOH:O	2.15	0.46
1:G:85:GLU:O	1:G:85:GLU:HG3	2.16	0.46
1:B:30:LEU:C	1:B:31:GLU:HG3	2.36	0.46
1:F:60:ASP:O	1:F:62:GLN:OE1	2.33	0.46
1:A:37:ILE:HG23	1:A:139:MSE:CE	2.46	0.46
1:B:34:GLY:HA3	1:B:180:TYR:CD1	2.49	0.46
1:F:148:ASP:OD2	1:H:84:GLU:OE2	2.33	0.46
1:C:107:TRP:CH2	1:C:163:MSE:HE1	2.52	0.45
1:E:78:PRO:CB	1:E:80:MSE:CE	2.93	0.45
1:F:49:MSE:HE1	1:F:145:LYS:HB2	1.98	0.45
1:B:80:MSE:CE	1:B:106:GLU:OE1	2.65	0.45
1:G:126:THR:CG2	1:G:128[A]:MSE:HE2	2.46	0.45
1:B:85:GLU:HG3	1:B:85:GLU:O	2.16	0.45
1:C:30:LEU:HD23	1:C:31:GLU:H	1.82	0.45
1:C:34:GLY:HA3	1:C:180:TYR:CE1	2.52	0.45
1:E:33:GLU:HB2	1:E:180:TYR:OH	2.16	0.45
1:G:34:GLY:HA3	1:G:180:TYR:CE1	2.52	0.45
1:G:37:ILE:HG23	1:G:139:MSE:CE	2.47	0.44
1:A:34:GLY:HA3	1:A:180:TYR:CE1	2.52	0.44
1:A:78:PRO:CG	1:A:80:MSE:CE	2.95	0.44
1:D:14:VAL:CG2	1:D:185:MSE:CE	2.94	0.44
1:F:49:MSE:HE3	1:H:82:ASP:CG	2.37	0.44
1:E:31:GLU:HA	1:E:32:GLY:HA2	1.74	0.44
1:F:49:MSE:HE3	1:H:82:ASP:HA	1.99	0.44
1:H:107:TRP:CH2	1:H:163:MSE:HE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLU:HA	1:B:195:GLU:OE1	2.18	0.44
1:D:154:ALA:HB3	1:D:192:VAL:HG11	2.00	0.44
1:F:107:TRP:CH2	1:F:163:MSE:HE1	2.53	0.44
1:F:30:LEU:HD13	1:F:176:THR:CG2	2.47	0.44
1:F:30:LEU:C	1:F:31:GLU:HG2	2.38	0.44
1:B:107:TRP:CH2	1:B:163:MSE:HE1	2.53	0.43
1:H:85:GLU:O	1:H:85:GLU:HG3	2.17	0.43
1:F:78:PRO:CG	1:F:80:MSE:CE	2.96	0.43
1:D:79:GLU:HG2	1:F:28:PRO:HD3	2.00	0.43
1:C:78:PRO:CG	1:C:80:MSE:CE	2.97	0.43
1:A:78:PRO:CG	1:A:80:MSE:HE3	2.49	0.43
1:B:37:ILE:HG23	1:B:139:MSE:CE	2.48	0.43
1:B:30:LEU:C	1:B:31:GLU:CG	2.88	0.42
1:D:49:MSE:HE2	1:D:79:GLU:OE2	2.18	0.42
1:G:61:MSE:HE3	3:G:346:HOH:O	2.14	0.42
1:A:125:LEU:HD13	1:A:126:THR:N	2.34	0.42
1:C:78:PRO:O	1:C:80:MSE:CE	2.66	0.42
1:C:31:GLU:HA	1:C:32:GLY:HA2	1.73	0.42
1:C:85:GLU:O	1:C:85:GLU:HG3	2.19	0.42
1:D:164:ASN:HA	1:D:164:ASN:HD22	1.72	0.42
1:H:33:GLU:HG2	1:H:58:ASN:ND2	2.34	0.42
1:A:78:PRO:O	1:A:80:MSE:CE	2.67	0.42
1:D:154:ALA:HB3	1:D:192:VAL:CG1	2.50	0.42
1:E:125:LEU:HD13	1:E:126:THR:N	2.35	0.42
1:G:8:ALA:O	1:G:10:LEU:HB2	2.18	0.42
1:G:65:MSE:CE	1:H:128[B]:MSE:HE1	2.50	0.42
1:D:37:ILE:HG23	1:D:139:MSE:CE	2.48	0.42
1:B:34:GLY:CA	1:B:180:TYR:CE1	2.99	0.41
1:E:164:ASN:HA	1:E:164:ASN:HD22	1.73	0.41
1:D:79:GLU:HG2	1:F:28:PRO:CD	2.49	0.41
1:B:6:VAL:HG22	1:B:117:GLU:OE1	2.19	0.41
1:D:78:PRO:O	1:D:80:MSE:CE	2.67	0.41
1:E:37:ILE:HG23	1:E:139:MSE:CE	2.48	0.41
1:E:78:PRO:O	1:E:80:MSE:CE	2.67	0.41
1:F:78:PRO:CG	1:F:80:MSE:HE3	2.50	0.41
1:F:85:GLU:O	1:F:85:GLU:HG3	2.19	0.41
1:B:125:LEU:HD13	1:B:126:THR:N	2.35	0.41
1:C:105:MSE:SE	1:D:167:LEU:HD21	2.71	0.41
1:F:9:ASP:HB2	1:F:21:ASN:HD21	1.86	0.41
1:G:128[B]:MSE:CG	1:H:128[B]:MSE:HE1	2.42	0.41
1:C:128:MSE:CE	1:D:101:GLY:HA3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HG23	1:C:139:MSE:CE	2.47	0.41
1:C:8:ALA:HB3	1:C:10:LEU:H	1.80	0.41
1:A:164:ASN:HA	1:A:164:ASN:HD22	1.73	0.41
1:D:78:PRO:CG	1:D:80:MSE:CE	2.98	0.41
1:F:31:GLU:HA	1:F:32:GLY:HA2	1.84	0.41
1:G:164:ASN:HA	1:G:164:ASN:HD22	1.72	0.41
1:G:33:GLU:HG2	1:G:58:ASN:ND2	2.36	0.41
1:C:14:VAL:CG2	1:C:185:MSE:HE1	2.51	0.41
1:G:31:GLU:HA	1:G:32:GLY:HA2	1.77	0.41
1:H:6:VAL:HG21	1:H:114:VAL:HA	2.03	0.41
1:A:33:GLU:HG2	1:A:58:ASN:ND2	2.36	0.40
1:B:164:ASN:HA	1:B:164:ASN:HD22	1.73	0.40
1:A:86:ARG:HD3	3:B:402:HOH:O	2.21	0.40
1:A:128:MSE:HE2	1:B:100:THR:O	2.21	0.40
1:D:14:VAL:CG2	1:D:185:MSE:HE3	2.51	0.40
1:F:78:PRO:HB2	1:F:80:MSE:HE2	2.02	0.40
1:G:128[B]:MSE:SE	1:H:101:GLY:HA3	2.72	0.40
1:F:78:PRO:O	1:F:80:MSE:CE	2.69	0.40
1:G:128[B]:MSE:HG2	1:H:128[B]:MSE:CE	2.44	0.40
1:H:31:GLU:HA	1:H:32:GLY:HA2	1.69	0.40
1:A:182:PHE:O	1:A:185:MSE:HG3	2.21	0.40
1:F:182:PHE:O	1:F:185:MSE:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/201 (96%)	186 (96%)	7 (4%)	0	100	100
1	B	191/201 (95%)	185 (97%)	6 (3%)	0	100	100
1	C	188/201 (94%)	180 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	189/201 (94%)	183 (97%)	6 (3%)	0	100 100
1	E	188/201 (94%)	183 (97%)	5 (3%)	0	100 100
1	F	192/201 (96%)	183 (95%)	8 (4%)	1 (0%)	29 34
1	G	191/201 (95%)	185 (97%)	6 (3%)	0	100 100
1	H	190/201 (94%)	185 (97%)	5 (3%)	0	100 100
All	All	1522/1608 (95%)	1470 (97%)	51 (3%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	197	HIS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	162/156 (104%)	158 (98%)	4 (2%)	47 60
1	B	161/156 (103%)	158 (98%)	3 (2%)	57 69
1	C	158/156 (101%)	154 (98%)	4 (2%)	47 60
1	D	159/156 (102%)	155 (98%)	4 (2%)	47 60
1	E	158/156 (101%)	156 (99%)	2 (1%)	69 80
1	F	162/156 (104%)	157 (97%)	5 (3%)	40 52
1	G	161/156 (103%)	156 (97%)	5 (3%)	40 52
1	H	160/156 (103%)	157 (98%)	3 (2%)	57 69
All	All	1281/1248 (103%)	1251 (98%)	30 (2%)	50 63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	173	ASN
1	B	125	LEU
1	B	164	ASN
1	B	173	ASN
1	C	11	ASN
1	C	30	LEU
1	C	75	ILE
1	C	164	ASN
1	D	125	LEU
1	D	164	ASN
1	D	191	THR
1	D	194	LEU
1	E	125	LEU
1	E	164	ASN
1	F	31	GLU
1	F	109	GLU
1	F	164	ASN
1	F	176	THR
1	F	197	HIS
1	G	5	SER
1	G	9	ASP
1	G	12	ASN
1	G	164	ASN
1	G	173	ASN
1	H	164	ASN
1	H	173	ASN
1	H	196	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	B	173	ASN
1	C	133	GLN
1	C	173	ASN
1	C	197	HIS
1	D	36	HIS
1	E	157	ASN
1	F	11	ASN
1	F	36	HIS
1	F	157	ASN

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Mol	Chain	Res	Type
1	F	164	ASN
1	G	173	ASN
1	H	157	ASN
1	H	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	184/201 (91%)	-0.22	11 (5%)	21	18	22, 30, 63, 95	0
1	B	182/201 (90%)	-0.17	8 (4%)	34	32	24, 37, 64, 125	0
1	C	179/201 (89%)	0.02	8 (4%)	33	30	27, 44, 92, 108	0
1	D	180/201 (89%)	0.41	14 (7%)	13	10	38, 57, 100, 126	0
1	E	179/201 (89%)	0.23	7 (3%)	39	36	40, 59, 86, 110	0
1	F	182/201 (90%)	0.06	12 (6%)	18	14	24, 45, 91, 132	0
1	G	181/201 (90%)	-0.37	2 (1%)	80	79	21, 30, 61, 90	0
1	H	180/201 (89%)	-0.22	5 (2%)	53	49	25, 37, 63, 114	0
All	All	1447/1608 (89%)	-0.03	67 (4%)	32	30	21, 42, 84, 132	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	7.9
1	F	8	ALA	7.7
1	B	4	SER	7.7
1	D	6	VAL	7.6
1	D	5	SER	6.8
1	H	196	HIS	5.9
1	E	6	VAL	5.8
1	B	5	SER	5.6
1	C	8	ALA	5.5
1	D	4	SER	5.5
1	A	10	LEU	5.4
1	A	2	GLY	5.3
1	D	31	GLU	5.2
1	F	7	THR	5.1
1	C	10	LEU	5.0
1	C	12	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	11	ASN	4.7
1	F	9	ASP	4.5
1	F	10	LEU	4.4
1	B	196	HIS	4.3
1	C	31	GLU	4.1
1	B	6	VAL	4.1
1	F	31	GLU	3.9
1	F	199	HIS	3.9
1	H	7	THR	3.8
1	C	11	ASN	3.6
1	F	11	ASN	3.6
1	A	196	HIS	3.5
1	D	7	THR	3.5
1	E	30	LEU	3.4
1	E	31	GLU	3.4
1	F	32	GLY	3.3
1	H	6	VAL	3.2
1	C	9	ASP	3.1
1	A	3	SER	3.0
1	C	32	GLY	2.9
1	C	197	HIS	2.9
1	B	195	GLU	2.9
1	E	7	THR	2.8
1	H	195	GLU	2.8
1	A	6	VAL	2.8
1	D	193	GLU	2.7
1	D	26	ASP	2.6
1	E	84	GLU	2.6
1	G	8	ALA	2.6
1	A	11	ASN	2.5
1	A	7	THR	2.4
1	A	5	SER	2.4
1	A	8	ALA	2.4
1	B	11	ASN	2.3
1	E	83	PRO	2.3
1	B	7	THR	2.3
1	D	33	GLU	2.3
1	A	9	ASP	2.3
1	F	174	ILE	2.3
1	D	45	LYS	2.3
1	D	9	ASP	2.2
1	F	197	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	4	SER	2.2
1	F	12	ASN	2.2
1	E	195	GLU	2.1
1	H	11	ASN	2.1
1	G	196	HIS	2.1
1	D	84	GLU	2.0
1	B	151	GLU	2.0
1	F	198	HIS	2.0
1	D	155	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	302	1/1	0.68	0.13	56,56,56,56	0
2	CL	B	301	1/1	0.91	0.20	71,71,71,71	0
2	CL	H	301	1/1	0.95	0.17	78,78,78,78	0
2	CL	A	301	1/1	0.98	0.12	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.